NAVSWC TR 91-250

(2)

ESTIMATION OF METAL ACCELERATION BY AN SF_5 CONTAINING EXPLOSIVE

BY HORST G. ADOLPH and G. WILLIAM LAWRENCE

RESEARCH AND TECHNOLOGY DEPARTMENT

30 JUNE1991

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FOREWORD

Interest has persisted in the SF_5 group as an oxidizing and property-modifying moiety for C, H, N, O explosive compounds. In the present report, cylinder expansion test results for an explosive containing an SF_5 compound are used to assess the ability of the SF_5 group to contribute to metal acceleration.

The authors thank P. Thomas and D. Remmers for the preparation of the charge. The SF_5 compound used in this work was prepared by M. Sitzmann.

The cylinder test was performed at the Los Alamos National Laboratory by I. Akst with the assistance of A. Gallegos, C. Martinez, and D. Hughes.

The work was funded by the Office of Naval Technology, Code 232, through the Explosives and Undersea Warheads Block.

Approved by:

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TABLES

INTRODUCTION

The purpose of the work described here was to obtain an estimate of the relative metal accelerating ability of an SF_5-containing explosive. The work is part of a continuing effort to assess the potential of the SF_5 moiety as an energetic group.[1,2] The approach taken was to perform a cylinder expansion test on a composition containing a significant amount of an SF_5 compound and to compare the results with the calculated performance of a corresponding composition containing an equal volume of an SF_5-free analog (H substituted for SF_5). A lack of heat of formation data on SF_5 compounds prevented calculation of the performance of the SF_5 composition and direct comparison with the experimental data.

The SF_5 compound and its H analog used in this work have the structures 1 and 2, respectively, and the properties listed below. Compound 2 was prepared by conversion of 3,6-dinitro-3,6-diazaoctane-1,8-diol to the bis(chlorocarbonate) followed by reaction with ammonia;[3] 1 was obtained by the literature procedure.[4]

$$\mathrm{SF_5NHCO\overset{\overset{O}{\|}}{C}H_2CH_2\overset{\overset{NO_2}{|}}{N}CH_2CH_2\overset{\overset{NO_2}{|}}{N}CH_2CH_2O\overset{\overset{O}{\|}}{C}NHSF_5}$$

1; $C_8H_{14}N_6O_8F_{10}S_2$

MP = 144-146°C
$\rho_o = 1.903\ g/cm^3$

$$\mathrm{H_2N\overset{\overset{O}{\|}}{C}OCH_2CH_2\overset{\overset{NO_2}{|}}{N}CH_2CH_2\overset{\overset{NO_2}{|}}{N}CH_2CH_2O\overset{\overset{O}{\|}}{C}NH_2}$$

2; $C_8H_{16}N_6O_8$

MP = 181-183°C
$\rho_o = 1.545\ g/cm^3$
$\Delta H_f = -231.8$ kcal/mol

The three compositions used in obtaining the performance estimate for 1 are shown in Table 1. These compositions were chosen because cylinder test data were available for the "baseline" composition, and partial substitution of the HMX by 2 and 1, respectively, provided suitable model compositions for evaluation of the SF_5 contribution.

TABLE 1. COMPOSITIONS USED FOR CYLINDER TEST AND CALCULATIONS

Ingredient	Composition	Baseline (13B/45)	Composition with 1 (CW1)	Composition with 2 (CW2)
HMX	wt%	78.15	58.63	60.89
	vol%	74.72	56.09	56.12
ADDITIVE 1 or 2	wt%	-	19.55	16.49
	vol%	-	18.70	18.69
FEFO	wt%	15.89	15.90	16.49
	vol%	18.10	18.10	18.11
FPF-1	wt%	5.30	5.30	5.50
	vol%	6.06	6.05	6.06
CURATIVE (DESMODUR N-100)	wt%	0.66	0.62	0.62
	vol%	1.13	1.07	1.03
DENSITY (g/cm^3)	TMD	1.818	1.818	1.751
	Actual (% TMD)	1.81 (99.6)	1.81 (99.6)	-

EXPERIMENTAL

The charge for the cylinder test was prepared as described earlier.[5] It was observed that 1 inhibited the cure of the FPF-1 binder with Desmodur N-100 polyisocyanate, but this was overcome with the use of a larger amount of cure catalyst (dibutyltin dilaurate) and a longer cure time. HMX classes 3, 4, and 5 in a ratio of 2.24:1:1 were used. The particle size of 1 was not determined but was probably in the range 50-150mm (i.e., neither very small nor very large).

The densities of 1 and 2 were determined by x-ray diffraction,* and the heat of formation of 2 was calculated from the heat of combustion.**

The loaded cylinder was radiographed to verify the quality of the charge and to aid in positioning the expansion-monitoring slit.[5] The cylinder test was performed and the data were evaluated at the Los Alamos National Laboratory as described previously.[5]

CALCULATIONS

Rather than risk a bias in a single computational method to calculate the cylinder energies needed for comparison with expermental data, it was decided to compare data from three known methods.

For the cylinder wall energy calculations with the KSM, a computer program was written based on the equations given in Reference 6.+

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*Unpublished work by R. Gilardi, Naval Research Laboratory, Washington, D. C.

**Determined by E. Baroody, Naval Ordnance Station, Indian Head, MD.

+The original definitions of N and M were expanded to accommodate the presence of fluorine in the composition.

Equations for cylinder wall energies in MJ/Kg, based on least squares correlation of calculated Isp and experimental cylinder wall energies, have since been added[7] to the equation for detonation pressure given for the GAB method in Reference 8. They are

$E(6mm) = 0.1272\ (Isp \times density)^{1.5} - 0.021$, and $E(19mm) = 0.1580\ (Isp \times density)^{1.5} + 0.007$,

where Isp is the specific impulse in newton-seconds/gram as calculated by the Propellant Evaluation Program[9] (PEP) and the density is in grams/cubic centimeter.

TIGER[10] calculations of cylinder energies were carried out according to procedures (written by Patricia Crawford of Lawrence Livermore National Laboratory, October 15, 1986) sent with the TIGER distribution package. These procedures outline a series of subroutines that can be called to compare the new material to a reference material. In this case, HMX was chosen for the reference material. The output from these subroutines can then be converted to cylinder wall energy.

RESULTS AND DISCUSSION

Table 2 shows the results of the cylinder test for the composition CW1, and the previously reported[5] data for the baseline composition. To evaluate the contribution of

TABLE 2. CYLINDER TEST RESULTS

Composition	Detonation Velocity- [km sec^{-1}]	Arrival Time [μsec]			Wall Velocity [km sec^{-1}]			Wall Energy [MJ/Kg]		
		6mm	19mm	30mm	6mm	19mm	30mm	6mm	19mm	30mm
CW1	8.13 ± 0.01	5.03	13.32	19.87	1.45	1.65	1.71	1.05	1.36	1.46
Baseline (13B/45)	8.50 ± 0.005	4.68	12.40	18.52	1.55	1.78	1.82	1.20	1.58	1.66

the SF_5 group to the observed cylinder wall acceleration, the wall energies for the baseline composition and for the composition CW2 were calculated by three different methods: KSM,[6] GAB,[8] and TIGER.[10] The results for CW2 were then corrected by the ratio of the experimental and calculated values for the baseline composition for each calculational method. These values for CW2 were then compared with the experimental

$$E(\text{corr.}) = E\,(\text{calc'd}) \quad \frac{E_{BASELINE}\,(\text{experimtl})}{E_{BASELINE}\,(\text{calc'd})}$$

values for CW1. The pertinent data are assembled in Table 3.

TABLE 3. CALCULATED AND EXPERIMENTAL CYLINDER WALL ENERGIES FOR COMPOSITIONS 13B/45, CW1, AND CW2

Composition / Wall Energy (MJ/Kg)	13B/45		CW1		CW2	
	6mm	19mm	6mm	19mm	6mm	19mm
Calc'd by KSM	1.30	1.62	-		1.10	1.38
Calc'd by GAB	1.23	1.56	-		1.03	1.32
Calc'd by TIGER	1.253	1.572	-		1.071	1.340
KSM value corr.	-		-		1.02	1.35
GAB value corr.	-		-		1.00	1.34
TIGER value corr.	-		-		1.026	1.35
Average of corrected values	-		-		1.015	1.35
Experimental	1.20	1.58	1.05	1.36	-	

Comparison of the average corrected value for the wall energies of CW2 with experimental values for CW1 shows the metal accelerating ability of the latter to be approximately equal or slightly greater.

ERROR ESTIMATES

The cylinder wall energies for CW1 may be uncertain to ±2% due to experimental error, although ±1% is considered more typical. The accuracy of the calculated average of corrected values for CW2 is more difficult to assess because not many experimental cylinder test data are available for similar compositions. Table 4 compares experimental wall energies for LX 09-0, RX 08-EL, Octol (78/22), LX 04, LX

TABLE 4. COMPARISON OF CALCULATED AND EXPERIMENTAL CYLINDER WALL ENERGIES FOR SOME HMX COMPOSITIONS*

Wall Energy (MJ/Kg) / Composition	ρ_o	Experimental		Calc'd by KSM		Calc'd by GAB		Calc'd by TIGER	
	g/cm^3	6mm	19mm	6mm (Δ,%)**	19mm (Δ,%)	6mm (Δ,%)	19mm (Δ,%)	6mm (Δ,%)	19mm (Δ,%)
LX 09-0	1.836	1.32	1.675	1.309 (0.8)	1.631 (2.6)	1.281 (3.0)	1.624 (3.0)	1.311 (0.7)	1.641 (2.0)
RX 08-EL	1.799	1.29	1.63	1.235 (4.3)	1.544 (5.3)	1.229 (4.7)	1.559 (4.4)	1.256 (2.6)	1.580 (3.1)
Octol (78/22)	1.813	1.215	1.535	1.218 (-.02)	1.521 (0.9)	1.193 (1.8)	1.514 (1.4)	1.210 (0.4)	1.519 (1.0)
LX 04	1.865	1.17	1.47	1.293 (-10.5)	1.601 (-8.9)	1.177 (-0.6)	1.496 (-1.8)	1.196 (-2.2)	1.485 (-1.0)
LX 07-1	1.857	1.250	1.575	1.336 (-6.9)	1.654 (-5.0)	1.227 (1.8)	1.558 (1.1)	1.263 (-1.0)	1.566 (0.6)
LX 10-0	1.862	1.315	1.670	1.380 (-4.9)	1.707 (-2.2)	1.286 (2.2)	1.630 (2.4)	1.325 (-0.8)	1.645 (1.5)

*Experimental Data from: B. M. Dobratz and P. C. Crawford, LLNL Explosives Handbook, UCRL 52997, Change 2, Jan 1985; P. C. Crawford, LLNL Cylinder Test Handbook, June 1987.

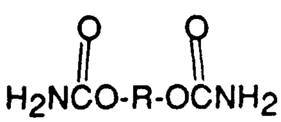
**Difference between experimental and calculated value.

07, and LX 10 with values calculated by the same three methods. It can be seen that for the explosives LX 09, RX 08-EL, and Octol, the calculations are mostly lower than experimental, while the explosives containing fluorinated binders (LX 04, LX 07, LX 10) tend to calculate higher (especially with KSM) than experimental. However, the averages of the GAB and TIGER values for the 3 fluorinated explosives are within +2% of experimental. Since CW2 contains a similar amount of fluorine, it is perhaps justified to assume that the GAB and TIGER calculated values for it are of similar uncertainty. On this basis, CW2 and CW1 are again about equal in performance.

CONCLUSIONS

The data presented above show the cylinder wall energy for CW1, the composition containing the SF_5 additive, to be 1.05 + 0.02 MJ/Kg at 6mm expansion and 1.36 $\pm$ 0.03 MJ/ Kg at 19mm expansion (standardized to 1" cylinder test). The analogous composition CW2, the composition with the inert additive, has calculated wall energies of 1.015 (6mm) and 1.35 (19mm) MJ/Kg. Based on the error estimates discussed above, the wall energies for the two compositions are essentially the same.

Because CW1 and CW2 contain only about 20% of the additives **1** or **2**, the performance of pure **1** and **2** could differ by as much as 10%. This compares with approximately 50% increase (based on KSM calculations) in performance when two hydrogens in **2** are replaced by two NO_2 groups to yield **3**. Thus, it is concluded that the SF_5 moiety will not be a major contributor to performance in metal acceleration, despite the large increase in density accompanying its presence. However, a small contribution is not ruled out by the present work.



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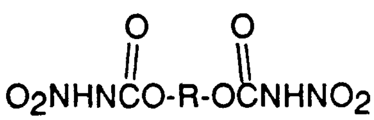

3

R = $CH_2CH_2N(NO_2)CH_2CH_2N(NO_2)CH_2CH_2$

ρ_o = 1.545 g/cm3
ΔH_f = -231.8 kcal/mol
E_{6mm} = 0.595 MJ/Kg
E_{19mm} = 0.767 MJ/Kg

ρ_o (calc'd) = 1.64 g/cm3
ΔH_f (calc'd) = -201 kcal/mol
E_{6mm} = 0.858 MJ/Kg
E_{19mm} = 1.103 MJ/Kg

As pointed out in reference 2, substitution of H by SF_5 (e.g., in a nitro compound) may have other beneficial effects such as desirable changes in melting point, glass transition temperature, vapor pressure, sensitivity, etc., which can justify the use of SF_5 in energetic molecules even if it is not a major energy carrier.

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GLOSSARY

HMX	N,N',N",N'"-Tetranitro-1,3,5,7-tetraazacyclooctane
FEFO	Bis(2,2,2-fluorodinitroethyl)formal
FPF-1	Poly(2,2,3,3,4,4-hexafluoropentanediol formal)
DESMODUR N-100	A trifunctional isocyanate obtained from MOBAY Chemical Corporation
KSM	Kamlet Short Method
GAB	Gill-Asaoka-Earoody
TIGER	A hydrodynamic-thermodynamic computer code for calculating detonation parameters
LX 09	HMX/Poly(2,2-dinitropropyl acrylate)/FEFO
RX 08-EL	HMX/FEFO/Polycaprolactone/Poly(vinyl formal)
OCTOL	HMX/TNT (78/22)
LX 04	HMX/VITON (85/15)
LX 07	HMX/VITON (90/10)
LX 10	HMX/VITON (95/5)

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4. TITLE AND SUBTITLE
Estimation of Metal Acceleration by an SF_5-Containing Explosive

5. FUNDING NUMBERS

6. AUTHOR(S)
Horst G. Adolph and G. William Lawrence

7. PERFORMING ORGANIZATION NAME(S) AND ADDRESS(ES)
Naval Surface Warfare Center
10901 New Hampshire Avenue
Silver Spring, Maryland 20903-5000

8. PERFORMING ORGANIZATION REPORT NUMBER
NAVSWC TR 91 -250

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800 N. Quincy Street
Arlington, VA 22217

10. SPONSORING/MONITORING AGENCY REPORT NUMBER

11. SUPPLEMENTARY NOTES

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Approved for public release; distribution unlimited.

12b. DISTRIBUTION CODE

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A two-inch cylinder expansion test was performed on a composition containing HMX, an energetic binder and 19 percent of a compound containing SF_5 groups. The experimental cylinder wall energies were compared with calculated data for an analogous composition devoid of SF_5. The results of this work suggest that replacing hydrogen by the SF_5 oxidizer moiety in a C,H,N,O explosive neither increases or decreases its metal accelerating ability substantially.

14. SUBJECT TERMS
Pentafluorosulfanyl Compounds Explosive Performance
Cylinder Expansion Test

15. NUMBER OF PAGES
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16. PRICE CODE

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